

ABSTRACT

There is provided a method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system. Measured isotope peak cluster data in a mass spectral range is obtained for a given calibration standard. Relative isotope abundances and actual mass locations of isotopes corresponding thereto are calculated for the given calibration standard. Mass spectral target peak shape functions centered within respective mass spectral ranges are specified. Convolution operations are performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data. A deconvolution operation is performed between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter.